

Author Search

=> FILE HCAPLUS

FILE 'HCAPLUS' ENTERED AT 08:37:01 ON 20 FEB 2008

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FILE COVERS 1907 - 20 Feb 2008 VOL 148 ISS 8

FILE LAST UPDATED: 19 Feb 2008 (20080219/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

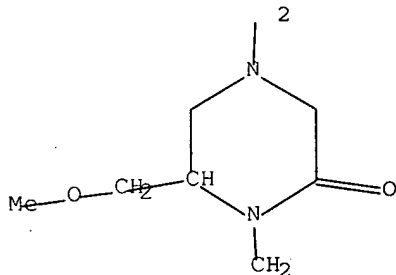
This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

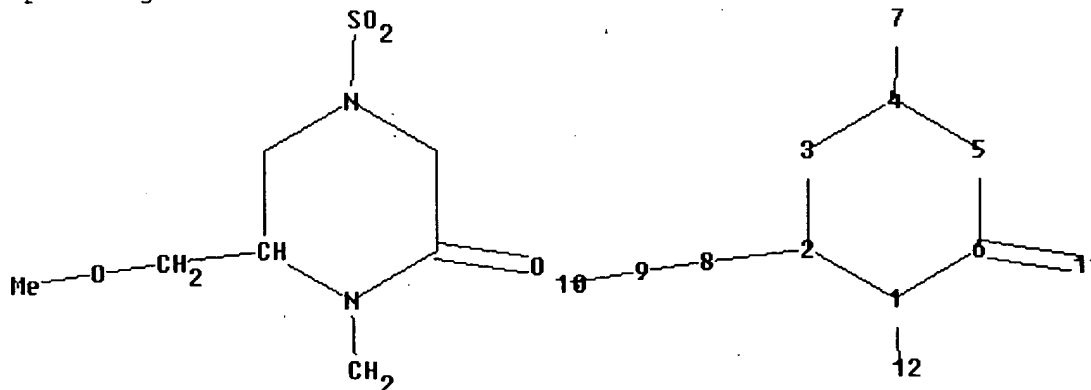
=> D QUE L32

L1

STR



Structure attributes must be viewed using STN Express query preparation:
Uploading strA.str



chain nodes :

7 8 9 10 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

1-12 2-8 4-7 6-11 8-9 9-10

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 6-11

exact bonds :

1-12 2-8 8-9 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

```

L2          41 SEA FILE=REGISTRY SSS FUL L1
L8 (        178)SEA FILE=HCAPLUS ABB=ON  PLU=ON  EWING W?/AU
L9 (        1692)SEA FILE=HCAPLUS ABB=ON  PLU=ON  BECKER M?/AU
L10 (        32)SEA FILE=HCAPLUS ABB=ON  PLU=ON  CHOI-SLEDESKI Y?/AU
L11 (        120)SEA FILE=HCAPLUS ABB=ON  PLU=ON  PAULS H?/AU
L12 (        170)SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONDON S?/AU
L13 (       3921)SEA FILE=HCAPLUS ABB=ON  PLU=ON  HE W?/AU
L14 (       6454)SEA FILE=HCAPLUS ABB=ON  PLU=ON  DAVIS R?/AU
L15 (        25)SEA FILE=HCAPLUS ABB=ON  PLU=ON  HANNEY B?/AU
L16 (       343)SEA FILE=HCAPLUS ABB=ON  PLU=ON  SPADA A?/AU
L17 (       740)SEA FILE=HCAPLUS ABB=ON  PLU=ON  BURNS C?/AU
L18 (      8035)SEA FILE=HCAPLUS ABB=ON  PLU=ON  JIANG J?/AU
L19 (      4707)SEA FILE=HCAPLUS ABB=ON  PLU=ON  LI A?/AU
L20 (     1097)SEA FILE=HCAPLUS ABB=ON  PLU=ON  MYERS M?/AU
L21 (      862)SEA FILE=HCAPLUS ABB=ON  PLU=ON  LAU W?/AU
L22 (      830)SEA FILE=HCAPLUS ABB=ON  PLU=ON  POLI G?/AU
L23 (       28)SEA FILE=HCAPLUS ABB=ON  PLU=ON  BOBKO M?/AU
L24 (     3128)SEA FILE=HCAPLUS ABB=ON  PLU=ON  MORRIS R?/AU
L25 (        0)SEA FILE=HCAPLUS ABB=ON  PLU=ON  KARPINSK J?/AU
L26 (     879)SEA FILE=HCAPLUS ABB=ON  PLU=ON  GALLAGHER T?/AU
L27 (       36)SEA FILE=HCAPLUS ABB=ON  PLU=ON  NEUENSCHWANDER K?/AU
L28 (       37)SEA FILE=HCAPLUS ABB=ON  PLU=ON  GRONEBERG R?/AU
L29 (       14)SEA FILE=HCAPLUS ABB=ON  PLU=ON  SABUCO J?/AU
L30      32941 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L8 OR L9 OR L10 OR L11 OR
          L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR
          L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR L28 OR L29)
L31          6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L2
L32          1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L30

```

=> D IBIB ED ABS FHITSTR L32 1

L32 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:78383 HCAPLUS Full-text

DOCUMENT NUMBER: 134:163059

TITLE: Substituted piperazinone derivatives and other
oxoazaheterocyclyl compounds useful as factor Xa/IIa
inhibitors

INVENTOR(S): Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls, Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Aiwen; Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.

PATENT ASSIGNEE(S): Aventis Pharmaceuticals Products Inc., USA

SOURCE: PCT Int. Appl., 460 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

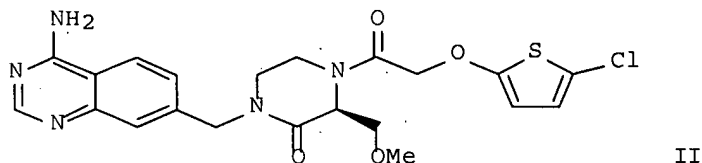
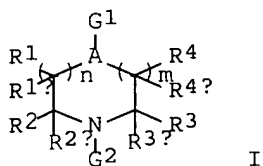
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007436	A2	20010201	WO 2000-IB1156	20000726
WO 2001007436	A3	20010823		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
CA 2382755	A1	20010201	CA 2000-2382755	20000726
BR 2000013179	A	20020402	BR 2000-13179	20000726
EP 1208097	A2	20020529	EP 2000-951781	20000726
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200225	T2	20020621	TR 2002-225	20000726
HU 2002003375	A2	20021228	HU 2002-3375	20000726
HU 2002003375	A3	20050329		
JP 2003508353	T	20030304	JP 2001-512520	20000726
EE 200200045	A	20030616	EE 2002-45	20000726
AU 773227	B2	20040520	AU 2000-64628	20000726
NO 2002000214	A	20020402	NO 2002-214	20020115
BG 106340	A	20021031	BG 2002-106340	20020122
ZA 2002000543	A	20030623	ZA 2002-543	20020122
MX 2002PA00888	A	20020730	MX 2002-PA888	20020125
PRIORITY APPLN. INFO.:			US 1999-363196	A 19990728
			WO 2000-IB1156	W 20000726

OTHER SOURCE(S): MARPAT 134:163059

ED Entered STN: 02 Feb 2001

GI



AB The invention is directed to piperazinones I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein A = CH or N; G1 and G2 = L1Cy1 or L2Cy2; Cy1 and Cy2 = (un)substituted aryl, heteroaryl, cycloalkyl, cycloalkenyl, heterocyclyl, etc.; L1 = null, O, S, SO, SO2, or (un)substituted sulfamoyl, methylene, (alkyl)keto(alkyl), carbamoyl, etc.; L2 = null or linking group; R1, R1a, R2, R2a, R3, R3a, R4, R4a = independently H, carboxy, alkoxycarbonyl, alkyl, (hetero)aryl, aralkyl, heteroarylalkyl, etc.; m and n = independently 0-2]. The compds. inhibit factor Xa (no data) and factor IIa, and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 1600 invention compds. and several hundred intermediates. For instance, condensation of 5-chloro-2-thienyloxyacetic acid with the corresponding N-benzyloxycarbonyl-protected piperazinone derivative (preps. given), using DIPEA and TBTU in DMF, gave II.

IT 323595-74-0P

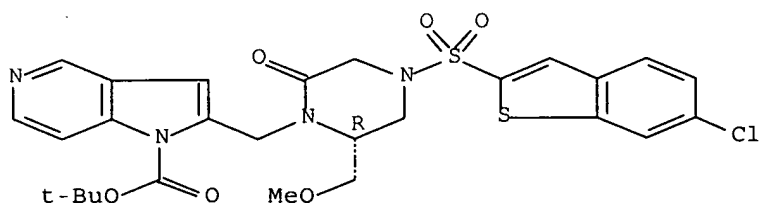
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa/IIa inhibitors)

RN 323595-74-0 HCAPLUS

CN 1H-Pyrrolo[3,2-c]pyridine-1-carboxylic acid, 2-[[[(2R)-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-2-(methoxymethyl)-6-oxo-1-piperazinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



Structure Search

=> FILE HCAPLUS

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FILE COVERS 1907 - 20 Feb 2008 VOL 148 ISS 8

FILE LAST UPDATED: 19 Feb 2008 (20080219/ED)

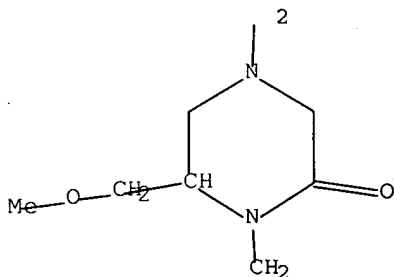
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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> D QUE L31

L1 STR



Structure attributes must be viewed using STN Express query preparation.

L2 41 SEA FILE=REGISTRY SSS FUL L1

L31 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L2

=> S L31 NOT L32

L47 5 L31 NOT L32

=> FILE MARPAT

FILE 'MARPAT' ENTERED AT 08:38:14 ON 20 FEB 2008

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FILE CONTENT: 1961-PRESENT VOL 148 ISS 6 (20080215/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2008004452	03	JAN	2008
DE	102006031314	03	JAN	2008
EP	1873224	02	JAN	2008
JP	2008001611	10	JAN	2008
WO	2008007169	17	JAN	2008
GB	2439172	19	DEC	2007
FR	2903012	04	JAN	2008
RU	2314304	10	JAN	2008
CA	2550557	14	DEC	2007

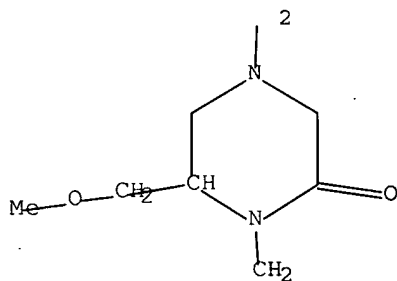
Expanded G-group definition display now available.

Effective December 15th the iteration and answer limits in MARPAT have increased from 100,000 to 200,000 for both on-line and batch searches. For more information on MARPAT search limits, type HELP SLIMITS at an arrow prompt.

=> D QUE L39

L1

STR



Structure attributes must be viewed using STN Express query preparation.

L38 10 SEA FILE=MARPAT SSS FUL L1

L39 10 SEA FILE=MARPAT ABB=ON PLU=ON L38/COM

=> FILE BEILSTEIN

FILE 'BEILSTEIN' ENTERED AT 08:38:29 ON 20 FEB 2008

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FILE LAST UPDATED ON January 3, 2008

FILE COVERS 1771 TO 2007.

*** FILE CONTAINS 10.119,480 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed

immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

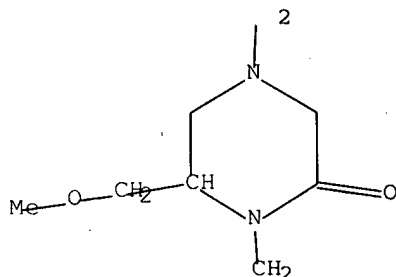
>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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*****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
*****
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>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

=> D QUE L45

L40 STR



Structure attributes must be viewed using STN Express query preparation.

```
L42      1 SEA FILE=BEILSTEIN SSS FUL L40
L43      1 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L42 AND BABSAN/FA
L45      0 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L42 NOT L43
```

=> FILE BABS

FILE 'BABS' ENTERED AT 08:38:38 ON 20 FEB 2008

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FILE LAST UPDATED: 3 JAN 2008 <20080103/UP>
FILE COVERS 1980 TO DATE.

=> D QUE L44

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L44      2 SEA FILE=BABS ABB=ON  PLU=ON  (6373992/BABSAN OR 6461519/BABSAN
      )
```

=> FILE WPIX

FILE 'WPIX' ENTERED AT 08:38:48 ON 20 FEB 2008
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FILE LAST UPDATED: 13 FEB 2008 <20080213/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200811 <200811/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of November 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and 20071130/UPIC. <<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
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http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:
http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0710.pdf

>>> XML document distribution format now available.

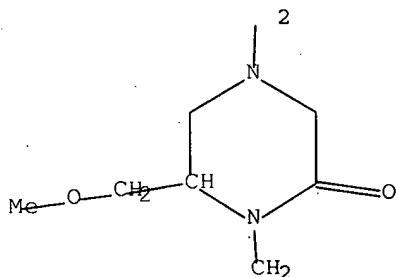
See HELP XMLDOC <<<

'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> D QUE L34

L1

STR



Structure attributes must be viewed using STN Express query preparation.
L34 0 SEA FILE=WPIX SSS FUL L1

=> DUP REM L47 L39 L45 L44 L34

L45 HAS NO ANSWERS

L34 HAS NO ANSWERS

DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE

FILE 'HCAPLUS' ENTERED AT 08:39:08 ON 20 FEB 2008

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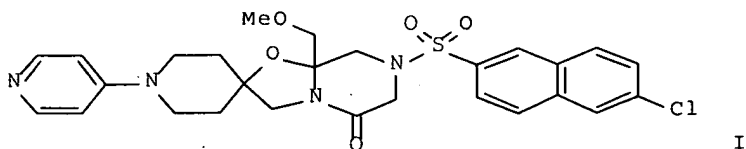
FILE 'MARPAT' ENTERED AT 08:39:08 ON 20 FEB 2008

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PROCESSING COMPLETED FOR L47
PROCESSING COMPLETED FOR L39
PROCESSING COMPLETED FOR L45
PROCESSING COMPLETED FOR L44
PROCESSING COMPLETED FOR L34
L48 12 DUP REM L47 L39 L45 L44 L34 (5 DUPLICATES REMOVED)
ANSWERS '1-5' FROM FILE HCAPLUS
ANSWERS '6-12' FROM FILE MARPAT

=> D IBIB ED ABS HITSTR L48 1-5; D IBIB AB QHIT 6-12

L48 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2004:336974 HCAPLUS Full-text
DOCUMENT NUMBER: 141:54295
TITLE: Synthesis and evaluation of 1-arylsulfonyl-3-piperazinone derivatives as factor Xa inhibitors IV. A series of new derivatives containing a spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-one skeleton
AUTHOR(S): Nishida, Hidemitsu; Mukaihira, Takafumi; Saitoh, Fumihiko; Harada, Kousuke; Fukui, Miyuki; Matsusue, Tomokazu; Okamoto, Atsushi; Hosaka, Yoshitaka; Matsumoto, Miwa; Shiromizu, Ikuya; Ohnishi, Shuhei; Mochizuki, Hidenori
CORPORATE SOURCE: Discovery Research Center, Mochida Pharmaceutical Co., Ltd., Shizuoka, 412-8524, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2004), 52(4), 406-412
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:54295
ED Entered STN: 26 Apr 2004
GI



AB In the course of development of factor Xa (FXa) inhibitors the title compds. were developed. Among such compds., (-)-7-[(6-chloro-2-naphthalenyl)sulfonyl]tetrahydro-8a-(methoxymethyl)-1'-(4-pyridinyl)-

spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-one (I, M55529) had IC50 2 nM, with high selectivity for FXa over thrombin and trypsin.

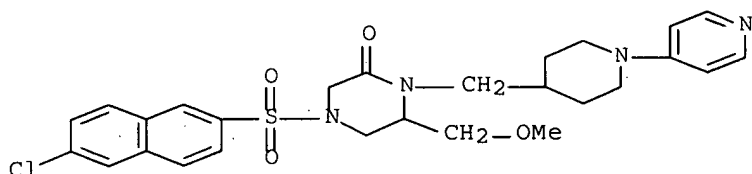
IT 229646-54-2

RL: PAC (Pharmacological activity); BIOL (Biological study)

(preparation of spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-ones as factor Xa inhibitors)

RN 229646-54-2 HCAPLUS

CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2002:256255 HCAPLUS Full-text

DOCUMENT NUMBER: 136:279479

TITLE: Preparation of piperazin-2-one amides as inhibitors of factor Xa

INVENTOR(S): Zhu, Bing-yan; Su, Ting; Li, Wenhao; Goldman, Erick A.; Zhang, Penglie; Jia, Zhaozhong Jon; Scarborough, Robert M.

PATENT ASSIGNEE(S): Cor Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 135 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026734	A1	20020404	WO 2001-US30313	20011001
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2422873	A1	20020404	CA 2001-2422873	20011001
AU 2002011280	A5	20020408	AU 2002-11280	20011001
EP 1322643	A1	20030702	EP 2001-979304	20011001
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BR 2001007282	A	20040706	BR 2001-7282	20011001

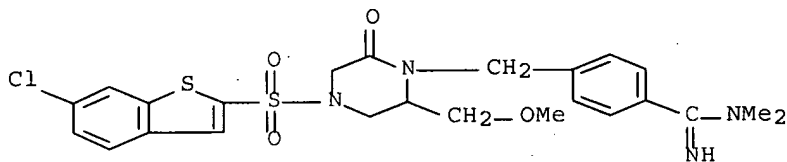
US 2004072860 A1 20040415 US 2003-381927 20030808
 PRIORITY APPLN. INFO.: US 2000-236393P P 20000929
 WO 2001-US30313 W 20011001
 OTHER SOURCE(S): MARPAT 136:279479
 ED Entered STN: 05 Apr 2002
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I or II; A = MeNHC(:NH), 1-methylimidazol-2-yl; PrNMeC(:NH), etc. R = H, alkyl, cycloalkyl, etc.; Q = III-VII; R1 = H, halo, alkyl, etc.; J1 = (un)substituted Ph, pyridyl, pyrimidinyl, furyl, thienyl; J2 = (un)substituted 2-naphthyl, 2-benzothienyl, etc.; n = 0-2; m = 1-2; p = 0-1], having activity against mammalian factor Xa (no data given), and useful in vitro or in vivo for preventing or treating conditions in mammals characterized by undesired thrombosis, were prepared E.g., a multi-step synthesis of VIII was given.

IT 406493-62-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of piperazin-2-one amides as inhibitors of factor Xa)

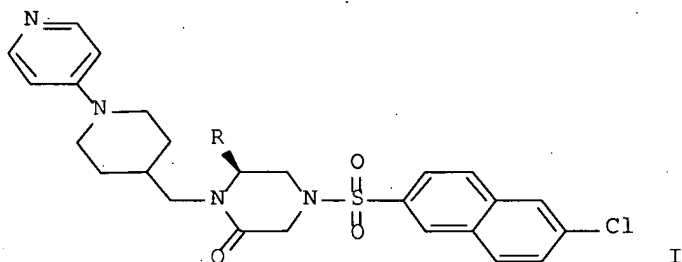
RN 406493-62-7 HCAPLUS
 CN Benzenecarboximidamide, 4-[[4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-2-(methoxymethyl)-6-oxo-1-piperazinyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 2002:723418 HCAPLUS Full-text
 DOCUMENT NUMBER: 138:137268
 TITLE: Synthesis and evaluation of 1-arylsulfonyl-3-piperazinone derivatives as factor Xa inhibitors II. Substituent effect on biological activities
 AUTHOR(S): Nishida, Hidemitsu; Miyazaki, Yutaka; Mukaihira, Takafumi; Saitoh, Fumihiko; Fukui, Miyuki; Harada, Kousuke; Itoh, Manabu; Muraoka, Aki; Matsusue, Tomokazu; Okamoto, Atsushi; Hosaka, Yoshitaka; Matsumoto, Miwa; Ohnishi, Shuhei; Mochizuki, Hidenori
 CORPORATE SOURCE: Chemistry Laboratory, Research Center, Mochida Pharmaceutical Co., Ltd., Shizuoka, 412-8524, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(9), 1187-1194
 CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:137268
 ED Entered STN: 24 Sep 2002
 GI



AB Intravascular clot formation is an important event in a number of cardiovascular diseases. The prevention of blood coagulation has become a major target for new therapeutic agents. Factor Xa (FXa) is a trypsin-like serine protease that plays a key role in the blood coagulation cascade and represents an attractive target for anticoagulant drug development. We have investigated substituents in the central part of a lead compound (I, R = H: M55113), and discovered that compound I (R = CO₂H: M55551 (R)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-oxo-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]-2-piperazinecarboxylic acid) is a potent inhibitor of FXa (IC₅₀=0.006 μM), with high selectivity for FXa over trypsin and thrombin. The activity of this compound is ten times more powerful than the lead compound

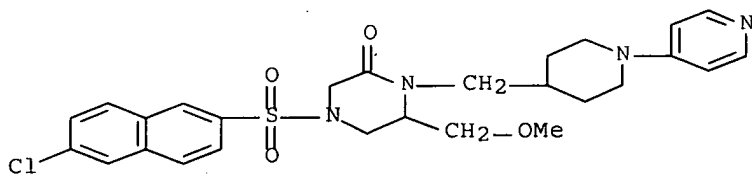
IT 229646-54-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, factor Xa inhibition, and structure-activity relationships of piperazinones via modifications on piperazinonecarboxylate)

RN 229646-54-2 HCAPLUS

CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



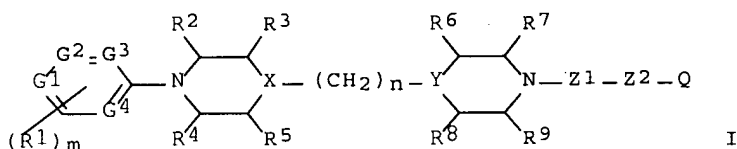
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 2001:12449 HCAPLUS Full-text
 DOCUMENT NUMBER: 134:71610

TITLE: Preparation of piperazine derivatives as cholesterol biosynthesis inhibitors
 INVENTOR(S): Nishida, Hidemitsu; Hosaka, Yoshitaka
 PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 130 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

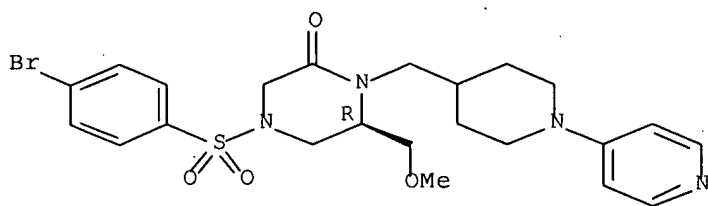
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000616	A1	20010104	WO 2000-JP4183	20000626
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: JP 1999-180879 A 19990625
 OTHER SOURCE(S): MARPAT 134:71610
 ED Entered STN: 05 Jan 2001
 GI



- AB The title compds. I [G1, G2, G3 and G4 are each independently CH or N, with the proviso that at least one of them is N; X and Y are each independently CH or N; Z1 is SO₂, CO or CH₂; Z2 is a single bond, lower alkylene, lower alkenylene or lower alkynylene; Q is optionally substituted aryl or optionally substituted heteroaryl; and n is an integer of 1 to 3; R1 = H, halo, carbamoyl, etc.; R2 - R5 = H, or CR₂, CR₃, CR₄, CR₅ = CO; R6 - R9 = H, alkoxy carbonyl, etc.; m = 0 - 3] are prepared I are useful as cholesterol biosynthesis inhibitors, particularly as 2,3-oxidosqualene cyclase inhibitors. In an in vitro test using cells, (R)-4-(4-bromobenzenesulfonyl)-6-ethoxycarbonyl-1-[1-(4-pyridyl)piperidin-4-ylmethyl]piperazin-2-one at 0.01 µg/mL gave 37% inhibition of cholesterol biosynthesis. Formulations are given.
- IT 314757-26-1P 314757-27-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of piperazine derivs. as cholesterol biosynthesis inhibitors)
- RN 314757-26-1 HCAPLUS
- CN Piperazinone, 4-[(4-bromophenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]-, (6R)- (9CI) (CA INDEX NAME)

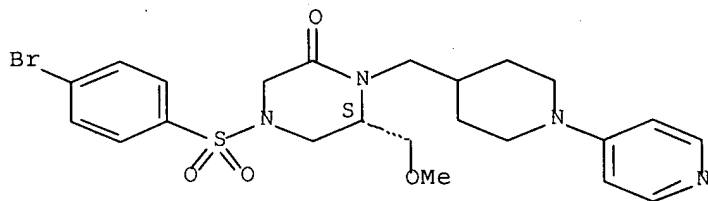
Absolute stereochemistry.



RN 314757-27-2 HCAPLUS

CN Piperazinone, 4-[[4-(4-bromophenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 1999:460402 HCAPLUS Full-text

DOCUMENT NUMBER: 131:87833

TITLE: Preparation of aromatic compounds having cyclic amino or salts thereof as FXa inhibitors

INVENTOR(S): Nishida, Hidemitsu; Hosaka, Yoshitaka; Miyazaki, Yutaka; Matsusue, Tomokazu; Mukaihira, Takafumi

PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 218 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933805	A1	19990708	WO 1998-JP6002	19981228
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,				

Serial No.:10/628,093

CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2318351	A1	19990708	CA 1998-2318351	19981228
AU 9916923	A	19990719	AU 1999-16923	19981228
EP 1048652	A1	20001102	EP 1998-961642	19981228

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

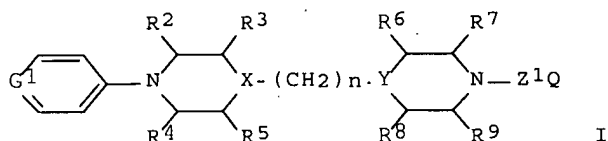
PRIORITY APPLN. INFO.:

JP 1997-367538	A	19971226
JP 1998-311491	A	19981030
WO 1998-JP6002	W	19981228

OTHER SOURCE(S): MARPAT 131:87833

ED Entered STN: 28 Jul 1999

GI



AB Title Comps. [I; G1, X and Y represent each CH or N; Z1 represents -SO2CH:CH- or -SO2-; Q represents aryl or heteroaryl; and R2 to R9 represent each hydrogen or a substituent; n = 0-1] and salts thereof which specifically inhibit FXa, exert a potent anticoagulant effect and thus are useful as medicinal comps. are prepared Title compound I (G1 = N; X = N; Y = CH; n = 0; R2 = H; R3 = H; R4 = H; R5 = H; R6 = H; R7 = H; R8 = H; R9 = H; Z1 = (E)-SO2CH:CH; Q = 4-ClC6H4) was prepared in two steps.

IT 229646-54-2P 229646-74-6P 229646-75-7P
229646-89-3P 229647-02-3P 229647-03-4P
229955-03-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

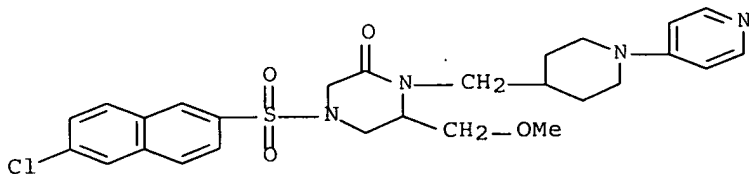
(preparation of aromatic comps. having cyclic amino or salts thereof as

FXa

inhibitors)

RN 229646-54-2 HCAPLUS

CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



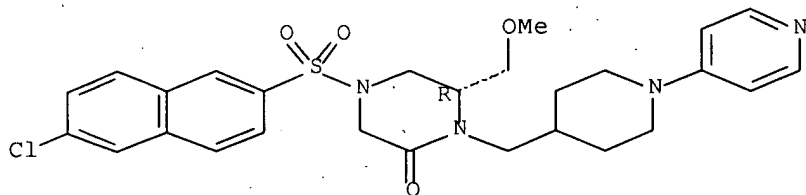
RN 229646-74-6 HCAPLUS

CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-

Serial No.:10/628,093

[[1-(4-pyridinyl)-4-piperidinyl]methyl]-, (6R)- (9CI) (CA INDEX NAME)

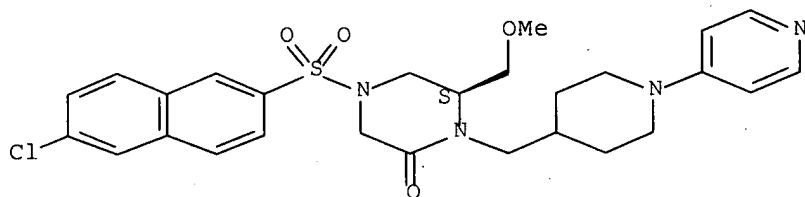
Absolute stereochemistry.



RN 229646-75-7 HCAPLUS

CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



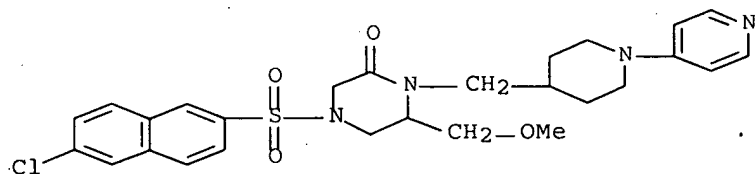
RN 229646-89-3 HCAPLUS

CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 229646-54-2

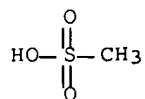
CMF C27 H31 Cl N4 O4 S



CM 2

CRN 75-75-2

CMF C H4 O3 S

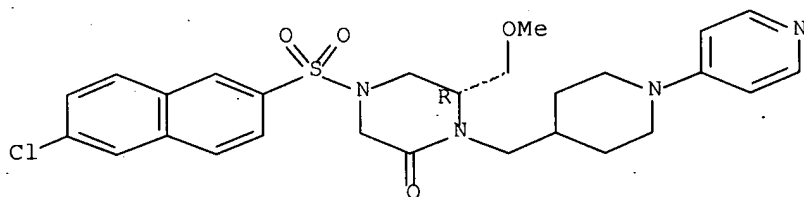


RN 229647-02-3 HCAPLUS
 CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-
 [[1-(4-pyridinyl)-4-piperidinyl]methyl]-, (6R)-, monomethanesulfonate
 (9CI) (CA INDEX NAME)

CM 1

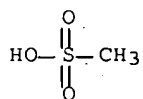
CRN 229646-74-6
 CMF C27 H31 Cl N4 O4 S

Absolute stereochemistry.



CM 2

CRN 75-75-2
 CMF C H4 O3 S

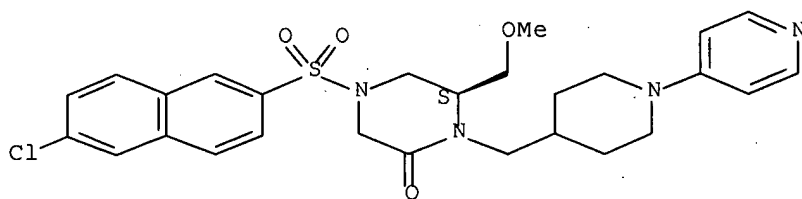


RN 229647-03-4 HCAPLUS
 CN Piperazinone, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-6-(methoxymethyl)-1-
 [[1-(4-pyridinyl)-4-piperidinyl]methyl]-, (6S)-, monomethanesulfonate
 (9CI) (CA INDEX NAME)

CM 1

CRN 229646-75-7
 CMF C27 H31 Cl N4 O4 S

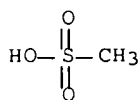
Absolute stereochemistry.



CM 2

CRN 75-75-2

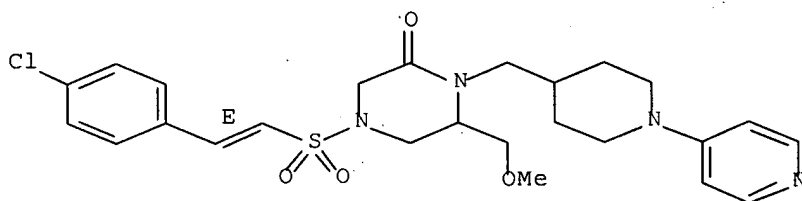
CMF C H4 O3 S



RN 229955-03-7 HCAPLUS

CN Piperazinone, 4-[[[(1E)-2-(4-chlorophenyl)ethenyl]sulfonyl]-6-(methoxymethyl)-1-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 6 OF 12 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:295962 MARPAT Full-text

TITLE: Preparation of benzodiazepine and benzopiperazine derivatives as inhibitors of histone deacetylase

INVENTOR(S): Leit, Silvana; Wahhab, Amal; Allan, Martin; Smil, David; Tessier, Pierre; Deziel, Robert; Chantigny, Yves Andre

PATENT ASSIGNEE(S): Methygene Inc., Can.

SOURCE: PCT Int. Appl., 161pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007022638	A1	20070301	WO 2006-CA1402	20060825
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

US 2007155730 A1 20070705

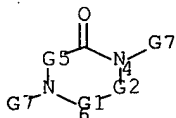
US 2006-467444 20060825

PRIORITY APPLN. INFO.:

US 2005-712011P 20050826

AB The title compds. with general formula I [wherein n = 0 or 1; U, V, W, and X = independently CH, N, or C-M, where no more than two of U, V, W, and X = N, and no more than one of U, V, W, and X = C-M; Y and Z = C=C, or when U, V, W, and X are absent, Y = a covalent bond and Z = CH₂ or CH(M), where M = independently halo, CF₃, NO₂, etc.; E and D = independently H, alkyl, heteroalkyl, etc.; A and B = independently H, alkyl, heteroalkyl, cycloalkyl, etc.] or N-oxides, hydrates, solvates, pharmaceutically acceptable salts, prodrugs, or complexes thereof were prepared as inhibitors of histone deacetylase in a cell. For example, compound II was prepared in a multi-step synthesis. II showed histone deacetylase enzyme inhibitory activity with IC₅₀ value of ≤ 50 nM.

MSTR 1A

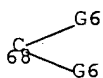


G1 = C(O)

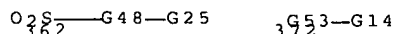
G2 = 66

⁶G⁸—⁶G⁹

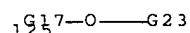
G5 = 68



G7 = 362 / 372



G8 = CH
G9 = 125



G17 = alkylene <containing 1-3 C>
G23 = alkyl <containing 1-6 C> (substd.)
G53 = carbon chain <containing 1-7 C, 0-1 double bond,
0-1 triple bond>

Patent location: claim 1
Note: and N-oxides, hydrates, solvates, pharmaceutically
acceptable salts, prodrugs and complexes
Note: substitution is restricted
Note: additional derivatization also claimed

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 7 OF 12 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:163140 MARPAT Full-text
TITLE: Heterocyclic sulfonamide derivatives as inhibitors of
Factor Xa, their preparation, pharmaceutical
compositions, and use in therapy
INVENTOR(S): Alstermark, Christer; Amin, Kosrat; Andersson, Kjell;
Fahlander, Ulf; Granberg, Kenneth; Hovdal, Daniel
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 85pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007008146	A1	20070118	WO 2006-SE840	20060705
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG,				

US, UZ, VC, VN, ZA, ZM, ZW
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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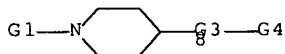
PRIORITY APPLN. INFO.:

SE 2005-1621

20050708

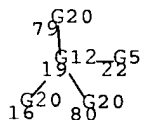
AB The invention relates to heterocyclic sulfonamides of formula I, which are inhibitors of Factor Xa. In compds. I, W, X, Y, and Z are independently selected from carbon and nitrogen, where at least one of W, X, Y, and Z is nitrogen and the bond between X and Y is a single bond or a double bond; n is 0-3; each R1 is independently H, halo, C1-3 alkyl, oxo, oxy, oxido, or thioxo; R2 is H or oxo; AB is CH₂CH₂ or CH=CH; m is 0-3; each R3 is independently selected from H, OH, oxo, C1-5 alkyl, carboxy, cyano, tetrazolyl, oxazolyl, C1-5 hydroxyalkyl, etc.; and R4 is H, halo, Me, or amino. The invention also relates to the preparation of compds. I, pharmaceutical compns. comprising a compound I and a pharmaceutically acceptable diluent or carrier, as well as to their use as antithrombotic or anticoagulant agents. Substitution of 6-chloro-2-methyl-2H-pyridazin-3-one with piperidine-4-carboxylic acid gave acid II, which was amidated with N-Boc-N'-allylethylenediamine and deprotected to give amine III. Sulfonylation of III with 1-benzenesulfonyl-3-chloro-1H-indole-6-sulfonyl chloride followed by deprotection, oxidation, and heterocyclization resulted in the formation of IV. The compds. of the invention are inhibitors of Factor Xa, e.g., compound IV expressed an IC₅₀ value of 4.8 nM in an anticoagulant activity assay.

MSTR 1

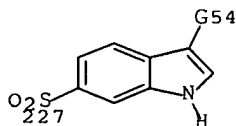


G3 = CH₂

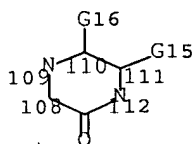
G4 = 19



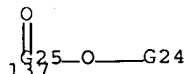
G5 = 227



G12 = 112-8 109-22 108-16 110-79 111-80



G20 = 137



G24 = alkyl <containing 1-5 C>

G25 = carbon chain <containing 1-5 C, saturated>

Patent location: claim 1

Note: or pharmaceutically acceptable salts

Note: substitution is restricted

Note: additional derivatization also claimed

Note: also incorporates claim 30

L48 ANSWER 8 OF 12 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:163137 MARPAT Full-text

TITLE: Heterocyclic sulfonamide derivatives as inhibitors of Factor Xa, their preparation, pharmaceutical compositions, and use in therapy

INVENTOR(S): Alstermark, Christer; Amin, Kosrat; Andersson, Kjell; Chen, Yantao; Fahlander, Ulf; Foote, Kevin Michael; Granberg, Kenneth; Hovdal, Daniel

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 127pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007008143	A1	20070118	WO 2006-SE837	20060705
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.:

SE 2005-1616

20050708

AB The invention relates to heterocyclic sulfonamides of formula I, which are inhibitors of Factor Xa. In compds. I, X is O or S; Y and Z are independently selected from carbon and nitrogen; n is 0, 1, or 2; each R1 is independently H or C1-3 alkyl; A and B are each selected from carbon and nitrogen, where at least one of A and B is nitrogen; R2 is H or oxo; L1 is an aliphatic, partially saturated, or aromatic carbocyclic ring containing 0, 1, or 2 nitrogen atoms; m is 0, 1, or 2; each R4 is independently selected from H, OH, oxo, C1-5 alkyl, carboxy, hydroxy-C1-5 alkyl, carboxy-C1-5 alkyl, carbamoyl, C1-5 alkylcarbamoyl, etc.; L2 is a bond, C1-4 alkylene, or C2-6 alkenylene; and R3 is optionally halo-substituted aryl ring containing 0, 1, or 2 heteroatoms. The invention also relates to the preparation of compds. I, pharmaceutical compns. comprising a compound I and a pharmaceutically acceptable diluent or carrier, as well as to their use as antithrombotic or anticoagulant agents. Substitution of 6-chloro-2-methyl-2H-pyridazin-3-one with piperidine-4-carboxylic acid gave acid II, which was amidated with N-Boc-N'-allylethylenediamine and deprotected to give amine III. Sulfonylation of III with 1-benzenesulfonyl-3-chloro-1H-indole-6-sulfonyl chloride followed by deprotection, oxidation, and heterocyclization resulted in the formation of IV. The compds. of the invention are inhibitors of Factor Xa, e.g., compound IV expressed an IC50 value of 4.8 nM in an anticoagulant activity assay.

MSTR 1

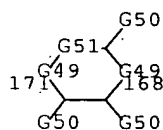
G1—S02—G44—G45

G1 = 4

G59—G7

G6 = CH2

G7 = 171-3 168-5



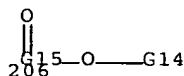
G14 = alkyl <containing 1-5 C>

G15 = carbon chain <containing 1-5 C, saturated>

G44 = bond

G49 = N

G50 = 206



G51 = C(O)
G59 = 283

~~224~~⁵—G4—~~283~~⁵

Patent location: claim 1
Note: substitution is restricted
Note: or pharmaceutically acceptable salts
Note: additional derivatization also claimed
Note: also incorporates claim 43

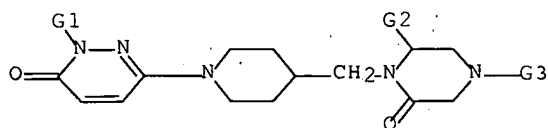
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 9 OF 12 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:163141 MARPAT Full-text
TITLE: Preparation of indolylsulfonyloxopiperazinylmethylpiperidinylpyridazinones as Factor Xa inhibitors.
INVENTOR(S): Alstermark, Christer; Andersson, Kjell; Fahlander, Ulf; Granberg, Kenneth
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 47pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

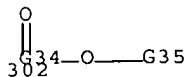
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007008142	A1	20070118	WO 2006-SE836	20060705
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PRIORITY APPLN. INFO.: SE 2005-1615 20050708
AB Title compds. [I; R1 = H, alkyl; R2 = OH, alkyl, carboxy, cyano, tetrazolyl, alkyltetrazolyl, oxazolyl, isoxazolyl, hydroxyalkyl, carboxyalkyl, alkoxyoxoalkyl, carbamoyl, alkylcarbamoyl, dialkylcarbamoyl, alkylcarbamoylalkyl, hydroxyalkylcarbamoyl, alkoxyalkylcarbamoyl, etc.; R3 = H, halo], were prepared Thus, iso-Pr 4-(3-chloro-1H-indole-6-sulfonyl)-1-[1-(1-methyl-6-oxo-1,6-dihydropyridazin-3-yl)piperidin-4-ylmethyl]-6-oxopiperazine-2-carboxylate (preparation given) inhibited Factor Xa with IC50 = 2.3 nM.

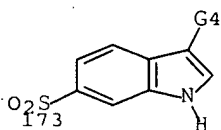
MSTR 1



G2 = 302



G3 = 173



G34 = carbon chain <containing 1-5 C, saturated>

G35 = alkyl <containing 1-5 C>

Patent location: claim 1

Note: or pharmaceutically acceptable salts

Note: also incorporates claim 10

Note: substitution is restricted

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 10 OF 12 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:332498 MARPAT Full-text

TITLE: Piperazine derivative and piperazinone derivative
inhibitors of factor Xa for the treatment of
cardiovascular disease

INVENTOR(S): Zhu, Bing-Yan; Zhang, Penglie; Goldman, Erick A.; Jia,
Zhaozhong Jon; Huang, Wenrong; Song, Yonghong; Su,
Ting; Scarborough, Robert M.; Wu, Yanhong

PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004032871 A2 20040422 WO 2003-US32117 20031008

WO 2004032871 A3 20040812

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003282566 A1 20040504 AU 2003-282566 20031008

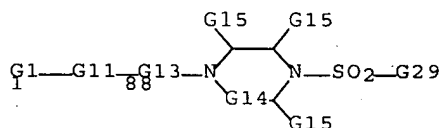
PRIORITY APPLN. INFO.:

US 2002-417474P 20021009

WO 2003-US32117 20031008

AB Piperazine and piperazinone inhibitors of factor Xa and a method of preparing such compds. are described. The use of such piperazinone compds. in the treatment of cardiovascular diseases is also described.

MSTR 1



G13 = CH2
 G14 = C(O)
 G15 = 372

³G₂¹⁸-G19

G18 = alkylene <containing 1-4 C>

G19 = alkoxy <containing 1-8 C>

Patent location: claim 1

Note: additional ring, ring oxo, and thioxo formation
 also claimed.

L48 ANSWER 11 OF 12 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 125:58998 MARPAT Full-text

TITLE: Purine and guanine compounds as inhibitors of purine
 nucleoside phosphorylase (pnp)

INVENTOR(S): Beasley, Steven Collin; Haughan, Alan Findlay;
 Montana, John; Watson, Robert John

PATENT ASSIGNEE(S): Chiroscience Limited, UK

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC: NUM. COUNT: 1

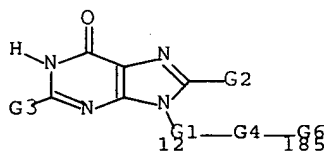
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9611200	A1	19960418	WO 1995-GB2363	19951005
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RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2201773	A1	19960418	CA 1995-2201773	19951005
AU 9536128	A	19960502	AU 1995-36128	19951005
AU 695032	B2	19980806		
ZA 9508397	A	19961007	ZA 1995-8397	19951005
EP 784624	A1	19970723	EP 1995-933490	19951005
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CN 1160402	A	19970924	CN 1995-195541	19951005
CN 1045088	B	19990915		
BR 9509236	A	19971021	BR 1995-9236	19951005
US 5736549	A	19980407	US 1995-539568	19951005
HU 77436	A2	19980428	HU 1997-1935	19951005
JP 10507171	T	19980714	JP 1995-512417	19951005
FI 9701413	A	19970404	FI 1997-1413	19970404
NO 9701538	A	19970604	NO 1997-1538	19970404
PRIORITY APPLN. INFO.:				
			GB 1994-20045	19941005
			GB 1994-20093	19941005
			GB 1994-20127	19941005
			WO 1995-GB2363	19951005

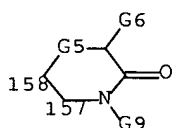
OTHER SOURCE(S): CASREACT 125:58998

AB Compds. of formula I, wherein n = 0-2, R1 = H, NH2, halogen, R2 = H, NH2, R3 is any of four ring systems, where m = 0 or 1, X = O, NR5, S(O)0-2, and may be different, R4 = H or one or more groups independently selected from C1-6-alkyl-R6 and aryl-R6, R5 = H, C1-6-alkyl-R6, C2-6-alkenyl, aryl, -aryl-C1-6-alkyl, -C1-6-alkyl-aryl, -C1-6-alkyl-hetero-C1-6-alkyl, CO2-C1-6-alkyl-R6, CONH-C1-6-alkyl-R6, CO-C1-6-alkyl-R6, SO2-C1-6-alkyl-R6, R6 = H, CO2H, CO2-C1-6-alkyl, COCONH2, CON(C1-6-alkyl)2, CHNH(C1-6-alkyl), CO-C1-6-alkyl, CO-aryl, CO-heteroaryl, tetrazolyl, NHSO2CF3, SO2NH-C1-6-alkyl, SO2N(C1-6-alkyl)2, SO2NH-aryl, NHCO-C1-6-alkyl, NHCONHC1-6-alkyl, NHCONH-aryl, NHSO2-C1-6-alkyl, NHSO2-aryl, CN, NH2, OH, O-C1-6-alkyl or O-aryl, in any tautomeric, salt, solvate and/or hydrate form, have utility as inhibitors of PNP.

MSTR 1



G1 = (0-2) CH2
 G4 = 158-12 157-185



G5 = 175

$$\text{N} \begin{array}{c} \text{175} \end{array} \text{---} \text{G9}$$

G6 = alkyl <containing 1-6 C> (opt. substd. by G7)

G7 = alkoxy <containing 1-6 C>

G9 = alkyl <containing 1-6 C> (opt. substd.) /
alkylsulfonyl <containing 1-6 C> (opt. substd.)

Derivative: and tautomers, salts, solvates, and/or hydrates

Patent location: claim 1

L48 ANSWER 12 OF 12 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 119:203434 MARPAT Full-textTITLE: Preparation of N-acyl-1-[(piperazinosulfonyl)methyl]bi
cycloheptyl(alkyl)amines and analogs as oxytocin
antagonistsINVENTOR(S): Bock, Mark G.; Erb, Jill M.; Hobbs, Doug W.; Hoffman,
James B.; Perlow, Debra S.; Pawluczyk, Joseph M.;
Veber, Daniel F.; Williams, Peter D.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: Eur. Pat. Appl., 142 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

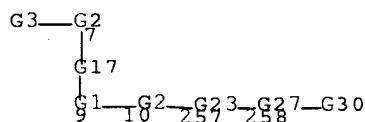
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 532097	A1	19930317	EP 1992-202689	19920905
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
WO 9306092	A1	19930401	WO 1992-US7214	19920826
W: BG, CS, FI, HU, NO, PL, RO, RU				
HU 67287	A2	19950328	HU 1994-738	19920826
CA 2077922	A1	19930314	CA 1992-2077922	19920910
AU 9223550	A	19930325	AU 1992-23550	19920911
AU 653059	B2	19940915		
CN 1070399	A	19930331	CN 1992-110672	19920911
ZA 9206936	A	19930428	ZA 1992-6936	19920911
JP 07242625	A	19950919	JP 1992-288091	19920914
JP 2523426	B2	19960807		
BR 9301159	A	19941018	BR 1993-1159	19930312
LT 3592	B	19951227	LT 1993-494	19930427
FI 9401136	A	19940310	FI 1994-1136	19940310
NO 9400882	A	19940311	NO 1994-882	19940311
US 5648352	A	19970715	US 1995-451779	19950526
PRIORITY APPLN. INFO.:			US 1991-759242	19910913

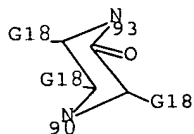
US 1992-917549	19920721
US 1991-760270	19910913
US 1991-760271	19910913
US 1991-760422	19910913
WO 1992-US7214	19920826
US 1992-993999	19921221
US 1992-995317	19921222
US 1993-40332	19930330
US 1994-179299	19940110

AB Title compds. I [R = bicycloalk(en)yl group Q1; R5, R6 = H, alkyl, phenylalkyl, etc.; R1, R8 = H, alkyl; R9, R10 = H, OH, halo, Me, etc.; R11 = H, NR12COR13, CONR14R15; R12 = H, alkoxy, alkyl, alkoxy carbonyl, etc.; R13 = H, alkoxy, CO2H, alkoxy carbonyl(amino), etc.; R14, R15 = H, alkyl, heterocyclyl, etc.; R16 = (substituted)Ph, -3-pyridyl; Y = CO, SO2; Z = bond, (carbonyl)alkylene; m, n = 0 or 1] were prepared. Thus, 1-(O-tolyl)piperazine was condensed with (+)-10-camphorsulfonyl chloride and the product condensed with EtCN to give, after reduction, I (R = bicycloheptyl group Q2, R5 = R = H, R16 = 2-MeC6H4, Y = SO2, m = 0, n = 1) (II; R17 = H) which was condensed with 4(5)-imidazoleacetic acid to give II [R17 = 4(5)-imidazoleacetyl]. The latter had an inhibiting concn.50 of 8 nM against oxytocin binding at rat uterus membrane preparation in vitro.

MSTR 1A

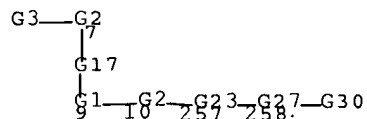


G1 = SO2
 G2 = (0-1) CH2
 G15 = alkoxy <containing 1-10 C>
 G17 = 93-7, 90-9

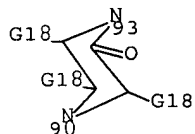


G18 = alkyl <containing 1-10 C>
 (opt. substd. by 1 or more G15)
 G27 = bond
 Derivative: or pharmaceutically acceptable salts
 Patent location: claim 1

MSTR 1B

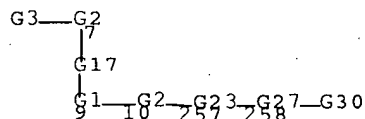


G1 = SO₂
 G2 = (0-1) CH₂
 G15 = alkoxy <containing 1-10 C>
 G17 = 93-7 90-9

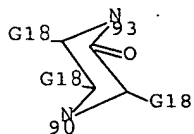


G18 = alkyl <containing 1-10 C>
 (opt. substd. by 1 or more G15)
 G27 = bond
 Derivative: or pharmaceutically acceptable salts
 Patent location: claim 1

MSTR 1C

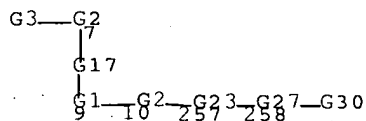


G1 = SO₂
 G2 = (0-1) CH₂
 G15 = alkoxy <containing 1-10 C>
 G17 = 93-7 90-9

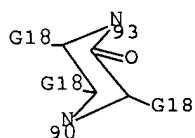


G18 = alkyl <containing 1-10 C>
 (opt. substd. by 1 or more G15)
 G27 = bond
 Derivative: or pharmaceutically acceptable salts
 Patent location: claim 1

MSTR 1D



G1 = SO₂
 G2 = (0-1) CH₂
 G15 = alkoxy <containing 1-10 C>
 G17 = 93-7 90-9



G18 = alkyl <containing 1-10 C>
 (opt. substd. by 1 or more G15)
 G27 = bond
 Derivative: or pharmaceutically acceptable salts
 Patent location: claim 1

Search History

L1 STR
 L2 41 SEA SSS FUL L1

 ACT SAC093RESEX/A

 L3 (1)SEA ABB=ON PLU=ON US2003-628093/APPS
 L4 SEL PLU=ON L3 1- RN : 1136 TERMS
 L5 (1136)SEA ABB=ON PLU=ON L4
 L6 (208)SEA ABB=ON PLU=ON L5 AND N>=2 AND O>=4
 L7 138 SEA ABB=ON PLU=ON L6 AND S>=1

FILE 'HCAPLUS' ENTERED AT 08:24:28 ON 20 FEB 2008
 ACT SAC093HC1AU/A

L8 (178)SEA ABB=ON PLU=ON EWING W?/AU
 L9 (1692)SEA ABB=ON PLU=ON BECKER M?/AU
 L10 (32)SEA ABB=ON PLU=ON CHOI-SLEDESKI Y?/AU
 L11 (120)SEA ABB=ON PLU=ON PAULS H?/AU
 L12 (170)SEA ABB=ON PLU=ON CONDON S?/AU
 L13 (3921)SEA ABB=ON PLU=ON HE W?/AU
 L14 (6454)SEA ABB=ON PLU=ON DAVIS R?/AU
 L15 (25)SEA ABB=ON PLU=ON HANNEY B?/AU
 L16 (343)SEA ABB=ON PLU=ON SPADA A?/AU
 L17 (740)SEA ABB=ON PLU=ON BURNS C?/AU
 L18 (8035)SEA ABB=ON PLU=ON JIANG J?/AU
 L19 (4707)SEA ABB=ON PLU=ON LI A?/AU
 L20 (1097)SEA ABB=ON PLU=ON MYERS M?/AU
 L21 (862)SEA ABB=ON PLU=ON LAU W?/AU
 L22 (830)SEA ABB=ON PLU=ON POLI G?/AU
 L23 (28)SEA ABB=ON PLU=ON BOBKO M?/AU
 L24 (3128)SEA ABB=ON PLU=ON MORRIS R?/AU
 L25 (0)SEA ABB=ON PLU=ON KARPINSK J?/AU
 L26 (879)SEA ABB=ON PLU=ON GALLAGHER T?/AU
 L27 (36)SEA ABB=ON PLU=ON NEUENSCHWANDER K?/AU
 L28 (37)SEA ABB=ON PLU=ON GRONEBERG R?/AU
 L29 (14)SEA ABB=ON PLU=ON SABUCO J?/AU
 L30 32941 SEA ABB=ON PLU=ON (L8 OR L9 OR L10 OR L11 OR L12 OR L13 OR
 L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR
 L23 OR L24 OR L25 OR L26 OR L27 OR L28 OR L29)

L31 6 SEA ABB=ON PLU=ON L2
 L32 1 SEA ABB=ON PLU=ON L31 AND L30

FILE 'WPIX' ENTERED AT 08:26:34 ON 20 FEB 2008

L33 0 SEA SSS SAM L1
 L34 0 SEA SSS FUL L1

FILE 'BEILSTEIN' ENTERED AT 08:29:45 ON 20 FEB 2008

L35 0 SEA ABB=ON PLU=ON L2
 L36 0 SEA ABB=ON PLU=ON L2

FILE 'MARPAT' ENTERED AT 08:31:53 ON 20 FEB 2008

L37 0 SEA SSS SAM L1
 L38 10 SEA SSS FUL L1
 L39 10 SEA ABB=ON PLU=ON L38/COM

FILE 'REGISTRY' ENTERED AT 08:32:31 ON 20 FEB 2008

L40

STRUCTURE UPLOADED

D

FILE 'BEILSTEIN' ENTERED AT 08:32:52 ON 20 FEB 2008

L41 0 SEA SSS SAM L40

L42 1 SEA SSS FUL L40

L43 1 SEA ABB=ON PLU=ON L42 AND BABSAN/FA
SEL BABSAN

FILE 'BABS' ENTERED AT 08:34:30 ON 20 FEB 2008

L44 2 SEA ABB=ON PLU=ON (6373992/BABSAN OR 6461519/BABSAN)

FILE 'BEILSTEIN' ENTERED AT 08:34:40 ON 20 FEB 2008

L45 0 SEA ABB=ON PLU=ON L42 NOT L43

FILE 'WPIX' ENTERED AT 08:35:46 ON 20 FEB 2008

L46 0 SEA SSS SAM L40

FILE 'HCAPLUS' ENTERED AT 08:37:27 ON 20 FEB 2008

D QUE L31

L47 5 SEA ABB=ON PLU=ON L31 NOT L32

FILE 'HCAPLUS, MARPAT, BABS' ENTERED AT 08:39:08 ON 20 FEB 2008

L48 12 DUP REM L47 L39 L45 L44 L34 (5 DUPLICATES REMOVED)